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Understanding GPCR allostery via Community network analysis

Gagan Jyot Kaur and Mukesh Chourasia

Amity Institute of Biotechnology,

Amity University Uttar Pradesh, Noida

gaganjyot12@gmail.com

G protein-coupled receptors (GPCRs) are one of the largest family of receptors present in humans. Their structure consists of 7 transmembrane helices which are connected by 3 intracellular and 3 extracellular loops. It has an extracellular N-terminal and an intracellular C-terminal. They are activated by various exogenous and endogenous ligands. Upon activation, a conformational change occurs in the receptor which activates the G-protein to trigger signaling. Therefore, GPCRs are allosteric proteins which sense the external signal and then respond intracellularly.

There are very few crystal structures of GPCRs which are available and also not much studies have been done on the receptor. This leads to many questions which need to be answered about the functional mechanism and dynamics of the receptor.

Our work focuses on conformational dynamics & allostery in GPCRs mainly Cannabinoid receptors. Earlier studies using Molecular dynamic simulations and Community network analysis have shown that there are subtle differences in the communication pathway from extracellular side to intracellular side upon various ligands binding in the orthosteric site.

This study will pave the way to design the ligands with specificity.

Keywords: GPCRs, Allostery, Community network, Molecular Dynamic Simulations.